Geometry of dynamics, Lyapunov exponents and phase transitions

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Abstract

The Hamiltonian dynamics of classical planar Heisenberg model is numerically investigated in two and three dimensions. In three dimensions peculiar behaviors are found in the temperature dependence of the largest Lyapunov exponent and of other observables related to the geometrization of the dynamics. On the basis of a heuristic argument it is conjectured that the phase transition might correspond to a change in the topology of the manifolds whose geodesics are the motions of the system.

On the basis of the ergodic hypothesis, Statistical Mechanics describes the physics of many-degrees of freedom systems by replacing *time* averages of the relevant observables with *ensemble* averages. In the present Letter, instead of using statistical ensembles, we investigate the Hamiltonian (microscopic) dynamics of a system undergoing a phase transition. The reason for tackling dynamics is twofold. First, there are observables, like Lyapunov exponents, that are intrinsically dynamical. Second, the geometrization of Hamiltonian dynamics in terms of Riemannian geometry provides new observables and, in general, a new interesting framework to investigate the phenomenon of phase transitions.

The geometrical formulation of the dynamics of conservative systems [1] was first used by Krylov in his studies on the dynamical foundations of statistical mechanics [2] and subsequently became a standard tool to study abstract systems in ergodic theory. Several new contributions to this subject appeared in the last years [3–6].

Let us briefly recall that the geometrization of the dynamics of N-degrees-of-freedom systems defined by a Lagrangian $\mathcal{L} = T - V$, in which the kinetic energy is quadratic in the velocities: $T = \frac{1}{2} a_{ij} \dot{q}^i \dot{q}^j$, stems from the fact that the natural motions are the extrema of the Hamiltonian action functional $\mathcal{S}_H = \int \mathcal{L}\, dt$, or of the Maupertuis' action $\mathcal{S}_M = 2 \int T\, dt$. In fact also the geodesics of Riemannian and pseudo-Riemannian manifolds are the extrema of a functional: the arc-length $\ell = \int ds$, with $ds^2 = g_{ij} dq^i dq^j$, hence a suitable choice of the metric tensor allows for the identification of the arc-length with either $\mathcal{S}_H$ or $\mathcal{S}_M$, and of the geodesics with the natural motions of the dynamical system. Starting from $\mathcal{S}_M$ the "mechanical manifold" is the accessible configuration space endowed with the Jacobi metric $(g_J)_{ij} = [E - V(\{q\})]\, a_{ij}$, where $V(q)$ is the potential energy and E is the total energy. A description of the extrema of Hamilton's action $\mathcal{S}_H$ as geodesics of a "mechanical manifold" can be obtained using Eisenhart's metric [7] on an enlarged configuration spacetime ($\{q^0 \equiv t, q^1, \ldots, q^N\}$ plus one real coordinate q^{N+1}), whose arc-length is

$$ds^2 = -2V(\mathbf{q})(dq^0)^2 + a_{ij} dq^i dq^j + 2 dq^0 dq^{N+1} \ . \qquad (1)$$

The manifold has a Lorentzian structure and the dynamical trajectories are those geodesics

satisfying the condition $ds^2 = Cdt^2$, where C is a positive constant. In the geometrical framework, the (in)stability of the trajectories is the (in)stability of the geodesics, and it is completely determined by the curvature properties of the underlying manifold according to the Jacobi equation [8]

$$\frac{D^2 J^i}{ds^2} + R^i_{\ jkm} \frac{dq^j}{ds} J^k \frac{dq^m}{ds} = 0 \ , \tag{2}$$

whose solution J, usually called Jacobi or geodesic variation field, locally measures the distance between nearby geodesics; D/ds stands for the covariant derivative along a geodesic and $R^i_{\ jkm}$ are the components of the Riemann curvature tensor. Using the Eisenhart metric (1) the relevant part of the Jacobi equation (2) is [4,6]

$$\frac{d^2 J^i}{dt^2} + R^i_{\ 0k0} J^k = 0 \ , \qquad i = 1, \dots, N \tag{3}$$

where the only non-vanishing components of the curvature tensor are $R_{0i0j} = \partial^2 V/\partial q_i \partial q_j$. Equation (3) is the tangent dynamics equation which is commonly used to measure Lyapunov exponents in standard Hamiltonian systems. Having recognized its geometric origin, in ref. [6] we have devised a geometric reasoning to derive from Eq.(3) an *effective* scalar stability equation that *independently* of the knowledge of dynamical trajectories provides an average measure of their degree of instability. This is based on two main assumptions: *i)* that the ambient manifold is *almost isotropic*, i.e. the components of the curvature tensor – that for an isotropic manifold (i.e. of constant curvature) are $R_{ijkm} = \kappa_0 (g_{ik} g_{jm} - g_{im} g_{jk})$, $\kappa_0 = const$ – can be approximated by $R_{ijkm} \approx \kappa(t)(g_{ik} g_{jm} - g_{im} g_{jk})$ along a generic geodesic $\gamma(t)$; *ii)* that in the large N limit the "effective curvature" $\kappa(t)$ can be modeled by a gaussian and δ-correlated stochastic process. The mean κ_0 and variance σ_κ of $\kappa(t)$ are given by the average and the r.m.s. fluctuation of the Ricci curvature $k_R = K_R/N$ along a geodesic: $\kappa_0 = \langle K_R \rangle / N$, and $\sigma_\kappa^2 = \langle (K_R - \langle K_R \rangle)^2 \rangle / N$ respectively. The Ricci curvature along a geodesic is defined as $K_R = R_{ij} \frac{dq^i}{dt} \frac{dq^j}{dt} / (\frac{dq^k}{dt} \frac{dq_k}{dt})$, where $R_{ij} = R^k_{\ ikj}$ is the Ricci tensor; in the case of Eisenhart metric it is $K_R \equiv \Delta V = \sum_{i=1}^N \partial^2 V / \partial q_i^2$. The final result is the replacement of Eq.(3) with the aforementioned effective stability equation which is independent of the dynamics and is in the form of a stochastic oscillator equation [5,6]

$$\frac{d^2\psi}{dt^2} + \kappa(t)\,\psi = 0 \ , \tag{4}$$

where $\psi^2 \propto |J|^2$. The exponential growth rate λ of the solutions of Eq. (4), which is therefore an estimate of the largest Lyapunov exponent, can be computed exactly:

$$\lambda = \frac{\Lambda}{2} - \frac{2\kappa_0}{3\Lambda}, \quad \Lambda = \left(2\sigma_\kappa^2\tau + \sqrt{\frac{64\kappa_0^3}{27} + 4\sigma_\kappa^4\tau^2}\,\right)^{\frac{1}{3}} \tag{5}$$

where $\tau = \pi\sqrt{\kappa_0}/(2\sqrt{\kappa_0(\kappa_0+\sigma_\kappa)} + \pi\sigma_\kappa)$; in the limit $\sigma_\kappa/\kappa_0 \ll 1$ one finds $\lambda \propto \sigma_\kappa^2$. Details can be found in Refs. [5,6].

In our geometric picture chaos is mainly originated by the parametric instability [9] activated by the fluctuating curvature "felt" by the geodesics. On the other hand, the average curvature properties are statistical quantities like thermodynamic observables. This means that there exists a non-trivial relationship between *dynamical* properties (Lyapunov exponents) and suitable *static* observables. Generic thermodynamic observables have a non-analytic behaviour as the system undergoes a phase transition. Hence the following question arises naturally: "Is there any peculiarity in the geometric properties associated with the dynamics, and thus in the chaotic dynamics itself, of systems which exhibit an equilibrium phase transition?" And in particular, do the curvature fluctuations and/or the Lyapunov exponent show any remarkable behaviour in correspondence with the phase transition itself? We address this question considering a system of planar classical "spins" (rotators) $\mathbf{S}_i = (\cos\varphi_i, \sin\varphi_i)$ defined on a d-dimensional lattice $\mathbb{Z}^d$. The Hamiltonian is

$$\mathcal{H}(\{\varphi,\pi\}) = \frac{1}{2}\sum_i \pi_i^2 + V(\{\varphi_i\}) \ , \tag{6}$$

where φ_i and π_i are the canonically conjugated angle and angular momentum of the "spin" on the i-th lattice site. The interaction is given by ($\langle ij\rangle$ stands for nearest-neighbour sites)

$$V = -\sum_{\langle ij\rangle\in\mathbb{Z}^d} \left(\cos(\varphi_i - \varphi_j) - 1\right) \ , \tag{7}$$

which is the Heisenberg XY potential. We consider $d = 2, 3$. The potential (7) is invariant under the action of the continuous group $O(2)$, hence — in the limit $N \to \infty$ — we expect

a second order phase transition only in $d = 3$ and a Kosterlitz-Thouless transition in $d = 2$. The equations of motion derived from the Hamiltonian (6) have been numerically integrated using a symplectic algorithm [10], with random initial conditions at equipartition (energy equally shared among the degrees of freedom) and at several values of the energy density $\varepsilon = E/N$. At each ε we measured the corresponding temperature T as the time average of the kinetic energy per degree of freedom. The temperature behavior of internal energy, specific heat and vorticity, computed as time averages instead of ensemble averages, led us to estimate a critical temperature $T_c \simeq 0.95$ in $d = 2$, in agreement with the already existing estimates [11], and $T_c \simeq 2.15$ in the $d = 3$ case. In Figs. 1 and 2 the values of the largest Lyapunov exponent, numerically computed using the standard algorithm [12], are plotted vs. the temperature T and are compared to their corresponding analytic estimates obtained by means of Eq. (5), where κ_0 and σ_κ are computed as time averages. The agreement between theoretical predictions and numerical data is very good; in an intermediate temperature range a "renormalization" of κ_0 is necessary, as already discussed in Ref. [6] for the one-dimensional case.

In the $d = 2$ case $\lambda_1(T)$ displays a rather smooth pattern in the transition region (see the inset of Fig. 1), whereas in the $d = 3$ case, at $T \simeq 2.15 \equiv T_c$, the behavior of $\lambda_1(T)$ clearly shows a neat departure from its intermediate regime of linear growth, as can be seen in the inset of Fig. 2 where the transition region is magnified and linear scales are used. No evidence of a possible divergence of $\lambda_1(T)$ is found as $T \to T_c$, at variance with the results reported in Ref. [13], though a very different model is considered therein. In this respect our results for $\lambda_1(T)$ are closer to those found for a liquid-solid first-order transition [14] and for other models [15].

Let us now turn to the *hidden* geometry of the dynamics and in particular to the complex landscape of the ambient manifold whose deviation from isotropy — quantified by σ_κ — is directly responsible for dynamical chaos. The comparison of Figs. 3 and 4, where $\kappa_0(T)$ and $\sigma_\kappa(T)$ are reported for $d = 2$ and $d = 3$ respectively, evidences a remarkable feature of the curvature fluctuations: a singular (cusp-like) behavior of $\sigma_\kappa(T)$ shows up in correspondence

with the second order phase transition and $\sigma_\kappa(T)$ is sharply peaked at T_c, whereas in absence of symmetry breaking ($d = 2$) no singular behaviour of $\sigma_\kappa(T)$ is present. This behavior of the curvature fluctuations is very intriguing. In fact a singular behavior of the curvature fluctuations can be reproduced in abstract geometric models which undergo a transition between different topologies at a critical value of a parameter that can be varied continuously. Let us consider for instance the families of surfaces of revolution immersed in $\mathbb{R}^3$ defined as follows: $\mathcal{F}_\varepsilon = (f_\varepsilon(u)\cos v, f_\varepsilon(u)\sin v, u)$, where u, v are local coordinates on the surface ($v \in [0, 2\pi]$ and u belongs to the domain of definition of f_ε), $f_\varepsilon(u) = \pm\sqrt{\varepsilon + u^2 - u^4}$, $\quad \varepsilon \in [\varepsilon_{\min}, +\infty)$, and $\varepsilon_{\min} = -\frac{1}{4}$. There is a critical value of the parameter, $\varepsilon = \varepsilon_c = 0$, corresponding to a change in the *topology* of the surfaces. In particular the manifolds $\mathcal{F}_\varepsilon$ are diffeomorphic to a torus $\mathbb{T}^2$ when $\varepsilon < 0$ and to a sphere $\mathbb{S}^2$ when $\varepsilon > 0$. Computing the Euler-Poincaré characteristic χ by means of the Gauss-Bonnet theorem [16], one finds $\chi(\mathcal{F}_\varepsilon) = 0$ if $\varepsilon < 0$, and $\chi(\mathcal{F}_\varepsilon) = 2$ otherwise.

Let M be a generic member of the family $\mathcal{F}_\varepsilon$, and let us define the fluctuations of the gaussian curvature K (see e.g. Ref. [16] for the definition of K) as $\sigma^2 = \langle K^2\rangle - \langle K\rangle^2 = A^{-1}\int_M K^2\, dS - A^{-2}(\int_M K\, dS)^2$ where A is the area of M and dS is the invariant surface element. This family of surfaces exhibits a singular behaviour in the curvature fluctuation σ as $\varepsilon \to \varepsilon_c$, as shown in Fig. 5. This is remarkably similar to the cusp-like behavior of the Ricci curvature fluctuations $\sigma_\kappa(T)$ of the XY model in $d = 3$ that are peaked at T_c [17]. At heuristic level, these results suggest that a phase transition might correspond to a *major topology change* in the manifolds underlying the motion. We conjecture that the family of "mechanical manifolds" (each one being in one-to-one correspondence with a value of T) splits, at T_c, into two subfamilies of manifolds that are not diffeomorphic (being perhaps of different cohomology type).

The relevance of topological concepts for the theory of phase transitions has been already rigorously demonstrated in a rather abstract context (see Ref. [18]); the present work suggests that also topological properties of the manifolds underlying the microscopic (Hamiltonian) dynamics could be relevant to second order phase transitions.

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REFERENCES

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[1] R. Abraham, J. E. Marsden, *Foundations of mechanics* (Addison-Wesley, Redwood City, 1987).

[2] N. S. Krylov, *Works on the foundations of statistical mechanics* (Princeton Univ. Press, Princeton, 1979).

[3] J. F. C. van Velsen, J. Phys. A **13**, 833 (1980); V. G. Gurzadyan and G. K. Savvidy, Astron. Astrophys. **160**, 203 (1986); H. Kandrup, Astrophys. J. **364**, 420 (1990); M. Szydlowski, J. Math. Phys. **35**, 1850 (1994); M. Szydlowski, M. Heller and W. Sasin, J. Math. Phys. **37**, 346 (1994); M. Szydlowski and A.Krawiec, Phys. Rev. D**53**, 6893 (1996).

[4] M. Pettini, Phys. Rev. E **47**, 828 (1993); L. Casetti and M. Pettini, Phys. Rev. E **48**, 2340 (1993); M. Cerruti-Sola and M. Pettini, Phys. Rev. E **51**, 53 (1995), and Phys. Rev. E **53**, 179 (1996); M. Pettini and R. Valdettaro, Chaos **5**, 646 (1995).

[5] L. Casetti, R. Livi, and M. Pettini, Phys. Rev. Lett. **74**, 375 (1995).

[6] L. Casetti, C. Clementi, and M. Pettini, Phys. Rev. E **54**, 5969 (1996).

[7] L. P. Eisenhart, Math. Ann. **30**, 591 (1929).

[8] M. P. do Carmo, *Riemannian geometry* (Birkhäuser, Boston-Basel, 1992).

[9] Parametric instability occurs when the parameters of a differential equation are suitably varied in time, see: V.I.Arnold, *Mathematical Methods of Classical Mechanics*, (Springer, New York, 1978).

[10] L. Casetti, Phys. Scripta **51**, 29 (1995).

[11] R. Gupta and C. F. Baillie, Phys. Rev. B**45**, 2883 (1992).

[12] G. Benettin, L. Galgani, and J.-M. Strelcyn, Phys. Rev. A **14**, 2338 (1976).

[13] A. Bonasera, V. Latora, and A. Rapisarda, Phys. Rev. Lett. **75**, 3434 (1995).

[14] Ch. Dellago, H. A. Posch, and W. G. Hoover, Phys. Rev. E **53**, 1485 (1996); Ch. Dellago and H. A. Posch, Physica A **230**, 364 (1996).

[15] P.Butera and G. Caravati, Phys. Rev. A**36**, 962 (1987); M. Antoni and S. Ruffo, Phys. Rev. E **52**, 2361 (1995).

[16] M. Spivak, *A comprehensive introduction to differential geometry* (Publish or Perish, Berkeley, 1979), Vol III.

[17] The values $\sigma_\kappa(T)$ are time averages instead of integrals over the "mechanical manifolds", but, despite a numerical trajectory usually samples a small part of the manifold, numerical time averages of σ_κ can give very good estimates of static averages (see ref. [6]).

[18] M. Rasetti, *Topological concepts in Phase Transition Theory*, in: *Differential Geometric Methods in Mathematical Physics*, C. Döbner, Ed. (Springer, New York, NY, 1990).

FIGURES

FIG. 1. Lyapunov exponent λ_1 vs. energy density ε for the $d = 2$ case. Numerical results correspond to lattice size: $N = 10^2$ (starred open squares), $N = 20^2$ (open triangles), $N = 40^2$ (open stars), $N = 50^2$ (open squares), $N = 100^2$ (open circles). Full squares are analytic results according to Eq.(4); dots are analytic results without correction (see text). In the inset symbols have the same meaning.

FIG. 2. Lyapunov exponent λ_1 vs. ε for the $d = 3$ case. Numerical results with lattice size: $N = 10^3$ (open squares), $N = 15^3$ (open star). Analytic results are represented by full circles; dots are analytic results without the correction mentioned in the text. Inset: $N = 10^3$ (open squares), $N = 15^3$ (open circles).

FIG. 3. $d = 2$ case. Time averages, at $N = 40^2$, of Ricci curvature (open circles) and its fluctuations (full circles). Solid lines are analytic estimates obtained from a high temperature expansion.

FIG. 4. $d = 3$ case. Time averages, at $N = 10^3$, of Ricci curvature (open triangles) and its fluctuations (full triangles). Open circles and full rhombs refer to a lattice size of $N = 15^3$. Solid lines are microcanonical analytic estimates obtained from a high temperature expansion. The appearence of a cusp-like behavior of curvature fluctuations is well evident at ε_c.

FIG. 5. Fluctuations amplitude, σ, of Gauss curvature of a family of surfaces parametrized by ϵ. For graphical reasons ϵ is shifted by its minimum value $|\epsilon_{min}| = 0.25$, thus the cusp corresponds to $\epsilon = 0$, the critical value separating two families of different Euler characteristic χ i.e. of different topology.

FIG. 1 Caiani et al.
''Geometry of Dynamics, Lyapunov Exponents...''

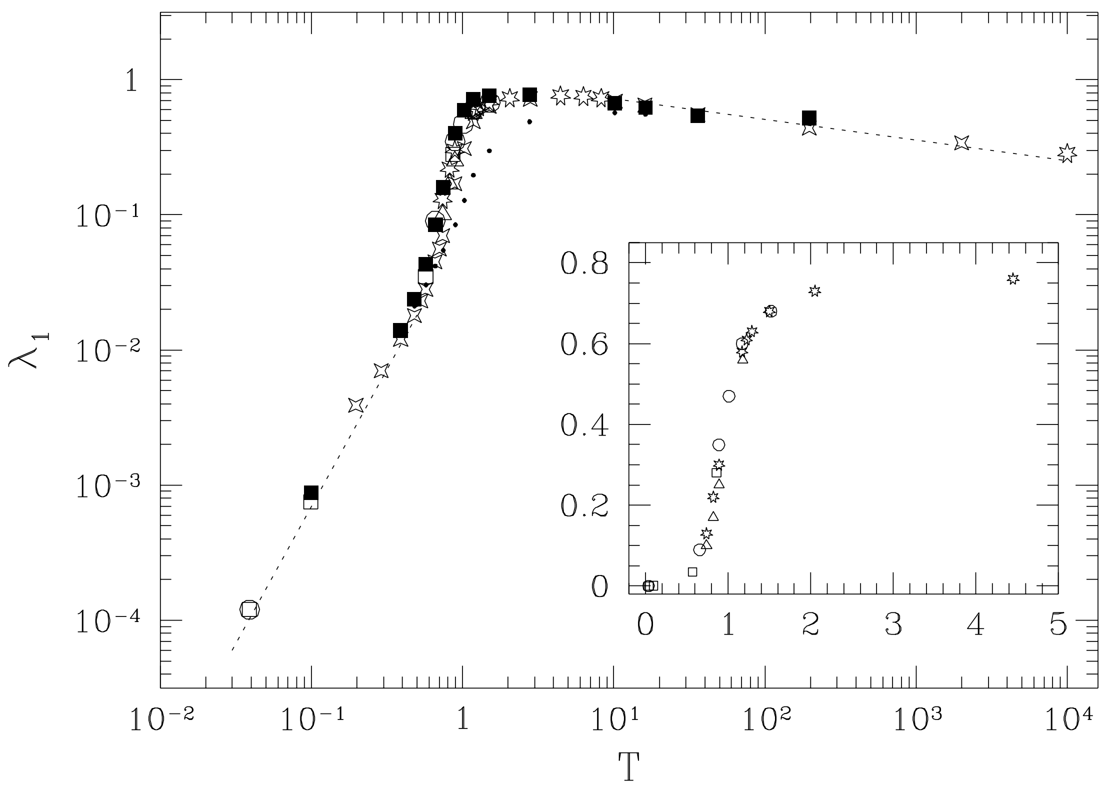

FIG. 2 Caiani et al.
"Geometry of Dynamics, Lyapunov exponents..."

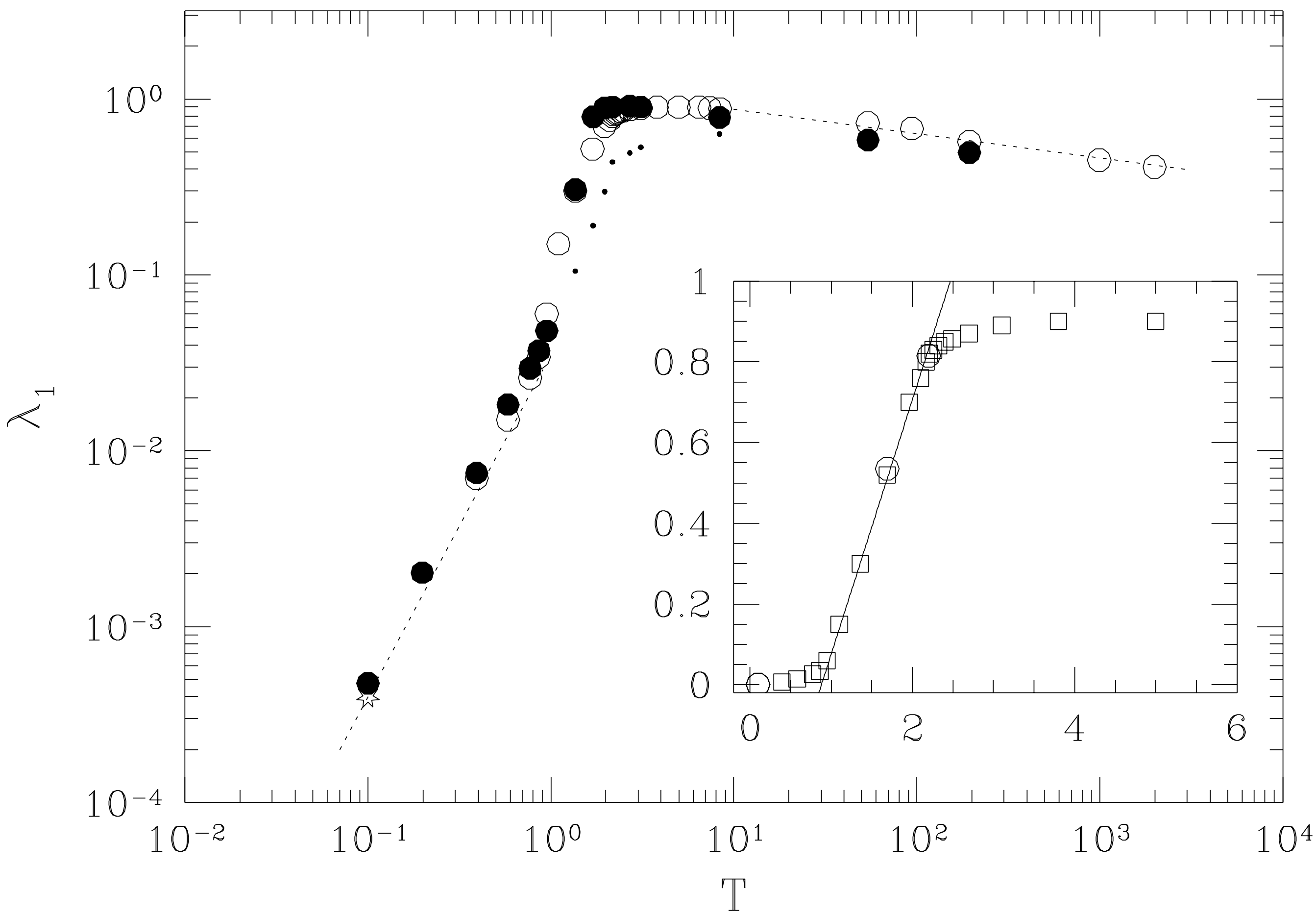

FIG. 3 Caiani et al.
''Geometry of Dynamics, Lyapunov Exponents...''

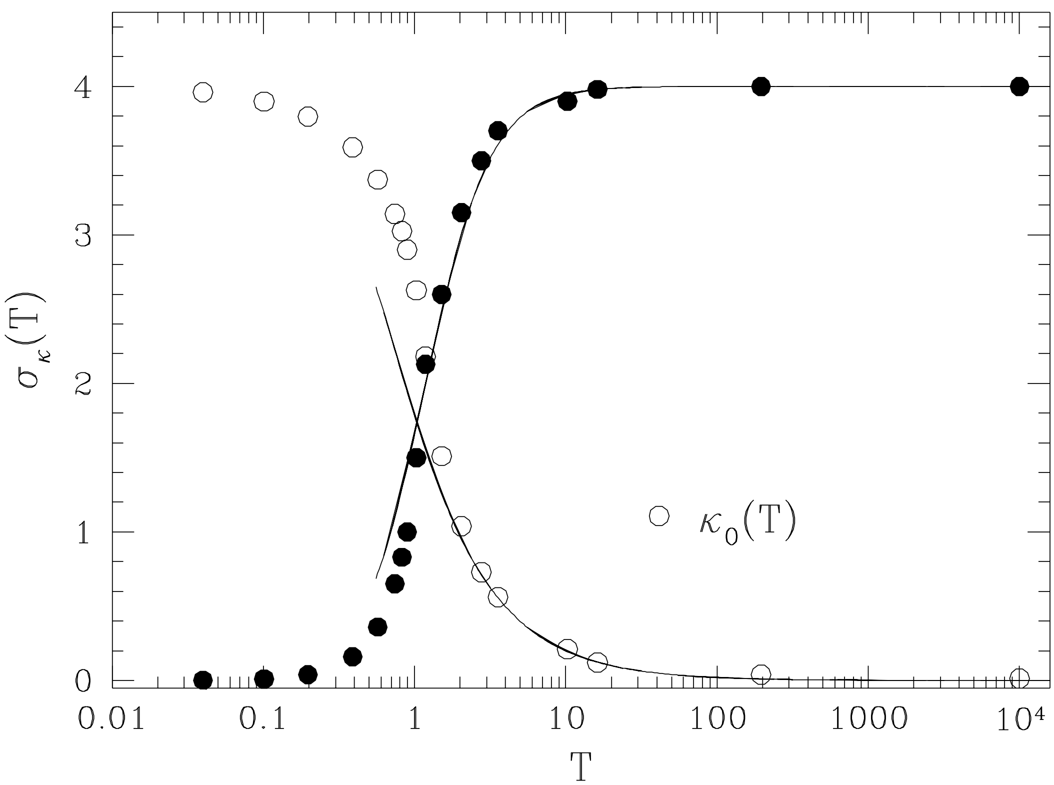

FIG. 4 Caiani et al.
''Geometry of Dynamics, Lyapunov Exponent...''

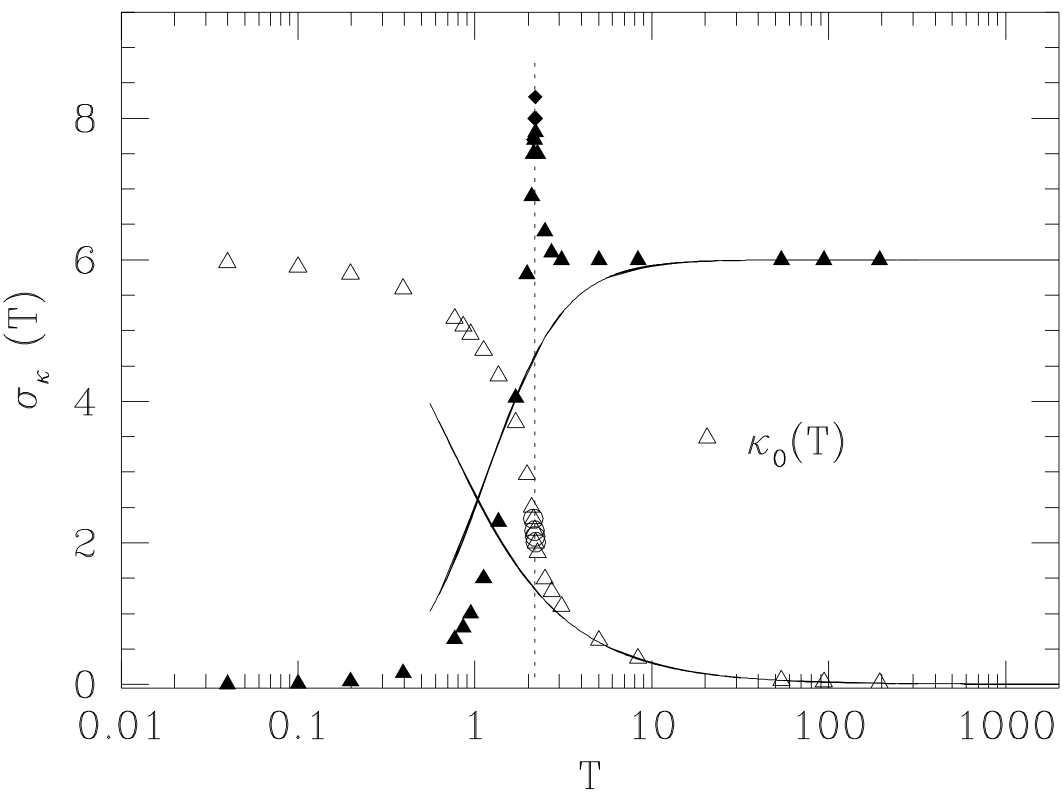

FIG. 5 Caiani et al.
''Geometry of Dynamics, Lyapunov Exponent...''